Package 'ADAPTS'

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Type Package

Title Automated Deconvolution Augmentation of Profiles for Tissue Specific Cells

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Description Augments existing or de-novo cell-type signature matrices to deconvolve bulk gene expression data.
Useful for building signature matrices from single cell RNAseq data, determine cell type deconvolution
spillover, and hierarchical deconvolution to use spillover to increase deconvolution accuracy. Please cite:
Danziger SA et al. (2019) ADAPTS: Automated Deconvolution Augmentation of Profiles for Tissue Specific cells <doi:10.1101/633958>. This package expands on the techniques outlined in Newman AM,
Liu CL, Green MR, Gentles AJ, Feng W, Xu Y,
Hoang CD, Diehn M, Alizadeh, AA (2015) <doi:10.1038/nmeth.3337>'s Nature Methods paper: 'Robust enumeration of cell subsets from tissue expression profiles' to allow a user to easily add their own cell types (e.g. a tumor specific cell type) to Newman's LM22 or other signature matrix.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

Depends R (>= 3.3.0)

biocViews

Imports missForest, e1071, WGCNA, ComICS, pheatmap, doParallel, quantmod, preprocessCore, pcaMethods, foreach, DeconRNASeq, nnls, ranger

Suggests R.rsp

VignetteBuilder R.rsp

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R topics documented:

AugmentSigMatrix . . . 3
buildSeed . . . 4
buildSpilloverMat . . . 6
calcAcc . . . 6
clustWspillOver . . . 7
collapseCellTypes . . . 8
estCellCounts.nPass . . . 9
estCellPercent . . . 9
estCellPercent.DCQ . . . 10
estCellPercent.DeconRNASeq . . . 12
estCellPercent.nnls . . . 13
estCellPercent.proportionsInAdmixture . . . 14
estCellPercent.spillOver . . . 15
estCellPercent.svmdecon . . . 16
getF1mcc . . . 17
getLM22cells . . . 18
gListFromRF . . . 18
hierarchicalClassify . . . 19
hierarchicalSplit . . . 20
Licenses . . . 21
LM22 . . . 22
loadMGSM27 . . . 23
loadModMap . . . 23
MGSM27 . . . 24
missForest.par . . . 25
plotKappas . . . 26
rankByT . . . 27
remakeLM22p . . . 28
scSample . . . 29
shrinkByKappa . . . 30
shrinkSigMatrix . . . 31
spillToConvergence . . . 32
splitSCdata . . . 33
SVMDECON . . . 34
weightNorm . . . 35

Index **36**

`AugmentSigMatrix` *Make an augmented signature matrix*

Description

Build an augmented signature matrix from an initial signature matrix, source data, and a list of differentially expressed genes (gList). The user might want to modify gList to make certain that particular genes are included in the matrix. The algorithm will be to add one additional gene from each new cell type Record the condition number, and plot those. Will only consider adding rows shared by fullData and newData

newMatData <- AugmentSigMatrix(origMatrix, fullData, newData, gList)

Usage

```
AugmentSigMatrix(
  origMatrix,
  fullData,
  newData,
  gList,
  nGenes = 1:100,
  plotToPDF = TRUE,
  imputeMissing = TRUE,
  condTol = 1.01,
  postNorm = FALSE,
  minSumToRem = NA,
  addTitle = NULL,
  autoDetectMin = FALSE,
  calcSpillOver = FALSE,
  pdfDir = tempdir()
)
```

Arguments

`origMatrix`	The original signature matrix
`fullData`	The full data for the signature matrix
`newData`	The new data to add signatures from
`gList`	The ordered list of genes from running rankByT() on newData. NOTE: best genes at the bottom!!
`nGenes`	The number of additional genes to consider (DEFAULT: 1:100)
`plotToPDF`	Plot the output condition numbers to a pdf file. (DEFAULT: TRUE)
`imputeMissing`	Set to TRUE to impute missing values. NOTE: adds stoachasiticity (DEFAULT: TRUE)
`condTol`	Setting higher tolerances will result in smaller numbers extra genes. 1.00 minimizes compliment number (DEFAULT: 1.00)

postNorm	Set to TRUE to normalize new signatures to match old signatures. (DEFAULT: FALSE)
minSumToRem	Set to non-NA to remove any row with the sum(abs(row)) < minSumToRem (DEFAULT: NA)
addTitle	An optional string to add to the plot and savefile (DEFAULT: NULL)
autoDetectMin	Set to true to automatically detect the first local minima. GOOD PRELIMINARY RESULTS (DEAFULT: FALSE)
calcSpillOver	Use the training data to calculate a spillover matrix (DEFAULT: FALSE)
pdfDir	A fold to write the pdf file to if plotToPDF=TRUE (DEFAULT: tempdir())

Value

an augmented cell type signature matrix

Examples

```
#This toy example treats the LM22 deconvolution matrix as if it were all of the data
#  For a real example, look at the vignette or comments in exprData, fullLM22, small LM22
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:200, 1:8]
#Make a fake signature matrix out of 100 genes and the first 8 cell types
smallLM22 <- fullLM22[1:100, 1:8]

#Make fake data representing two replicates of purified Mast.cells
exprData <- ADAPTS::LM22[1:200, c("Mast.cells.resting","Mast.cells.activated")]
colnames(exprData) <- c("Mast.cells", "Mast.cells")

#Fake source data with replicates for all purified cell types.
#  Note in this fake data set, many cell types have exactly one replicate
fakeAllData <- cbind(fullLM22, as.data.frame(exprData))
gList <- rankByT(geneExpr = fakeAllData, qCut=0.3, oneCore=TRUE)

newSig <- AugmentSigMatrix(origMatrix=smallLM22, fullData=fullLM22, newData=exprData,
    gList=gList, plotToPDF=FALSE)
```

---

buildSeed *Build a deconvolution seed matrix*

Description

Use ranger to select features and build a genesInSeed gene matrix

Usage

```
buildSeed(
  trainSet,
  genesInSeed = 200,
```

```
  groupSize = 30,
  randomize = TRUE,
  num.trees = 1000,
  plotIt = FALSE,
  trainSet.3sam = NULL,
  trainSet.30sam = NULL
)
```

Arguments

trainSet	Each row is a gene, and each column is an example of a particular cell type, ie from single cell data
genesInSeed	The maximum number of genes in the returned seed matrix (DEFAULT: 200)
groupSize	The number of groups to break the trainSet into by ADAPTS::scSample (DEFAULT: 30)
randomize	Set to TRUE randomize the sets selected by ADAPTS::scSample (DEFAULT: TRUE)
num.trees	The number of trees to be used by ranger (DEFAULT: 1000)
plotIt	Set to TRUE to plot (DEFAULT: FALSE)
trainSet.3sam	Optional pre-calculated ADAPTS::scSample(trainSet, groupSize = 3) (DEFAULT: NULL)
trainSet.30sam	Optional pre-calculated ADAPTS::scSample(trainSet, groupSize=groupSize, randomize=randomize) (DEFAULT: NULL)

Value

A list with condition numbers and gene lists

Examples

```
library(ADAPTS)
ct1 <- runif(1000, 0, 100)
ct2 <- runif(1000, 0, 100)
dataMat <- cbind(ct1, ct1, ct1, ct1, ct1, ct1, ct2, ct2, ct2, ct2)
rownames(dataMat) <- make.names(rep('gene', nrow(dataMat)), unique=TRUE)
noise <- matrix(runif(nrow(dataMat)*ncol(dataMat), -2, 2), nrow = nrow(dataMat), byrow = TRUE)
dataMat <- dataMat + noise
newSigMat <- buildSeed(trainSet=dataMat)
```

buildSpilloverMat *Build a spillover matrix*

Description

Build a spillover matrix, i.e. what do purified samples deconvolve as?

spillExpr <- buildSpilloverMat(refExpr, geneExpr, method='DCQ')

Usage

```
buildSpilloverMat(refExpr, geneExpr, method = "DCQ")
```

Arguments

refExpr	The deconvolution matrix, e.g. LM22 or MGSM27
geneExpr	The full gene expression for purified cell types. Multiple columns (examples) for each column in the reference expr.
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)

Value

A spillover matrix showing how purified cell types deconvolve

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

spillover <- buildSpilloverMat(refExpr=smallLM22, geneExpr=fullLM22, method='DCQ')
```

calcAcc *Calculate prediction accuracy*

Description

Calculate correlation coeffifients, p-Values, MAE, RMSE for deconvolution predictions

Usage

```
calcAcc(estimates, reference)
```

Arguments

estimates	The estimated cell percentages
reference	The reference cell percentages

Value

a list with a multiple sets

Examples

```
estimates <- sample(c(runif(8), 0 ,0))
estimates <- 100 * estimates / sum(estimates)
reference <- sample(c(runif(7), 0 , 0, 0))
reference <- 100 * reference / sum(reference)
calcAcc(estimates, reference)
```

---

clustWspillOver *Cluster with spillover*

Description

Build clusters based on n-pass spillover matrix

Usage

```
clustWspillOver(
  sigMatrix,
  geneExpr,
  nPasses = 100,
  deconMatrices = NULL,
  method = "DCQ"
)
```

Arguments

sigMatrix	The deconvolution matrix, e.g. LM22 or MGSM27
geneExpr	The source gene expression matrix used to calculate sigMatrix.
nPasses	The maximum number of iterations for spillToConvergence (DEFAULT: 100)
deconMatrices	Optional pre-computed results from spillToConvergence (DEFAULT: NULL)
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)

Value

Cell types grouped by cluster

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

clusters <- clustWspillOver(sigMatrix=smallLM22, geneExpr=fullLM22, nPasses=10)
```

`collapseCellTypes` *Collapse cell types*

Description

Collapse the cell types (in rows) to super-classes Including MGSM36 cell types

Usage

```
collapseCellTypes(cellCounts, method = "Pheno4")
```

Arguments

`cellCounts`	A matrix with cell counts
`method`	The method for combining cell types ('Default: 'Pheno2') Pheno1: Original cell-type based combinations Pheno2: Original cell-type based combinations, omitting Macrophages Pheno3: Alt Phenotype definitions based on WMB deconvolution correlations Pheno4: Consensus cell types Pheno5: Consensus cell types, combined myeloma & plasma Spillover1: Empirical combinations based on compToLM22source Spillover2: More agressive combination based on empirical combinations based on compToLM22source Spillover3: Combinations determined by spillToConvergence on 36 cell types

Value

a cell estimate matrix with the names changed

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.DCQ(refExpr=smallLM22, geneExpr=fullLM22)
collapseCounts <- collapseCellTypes(cellCounts=cellEst)
```

`estCellCounts.nPass` *Deconvolve with an n-pass spillover matrix*

Description

curExpr <- estCellCounts.nPass(sigMatrix, deconMatrices)

Usage

```
estCellCounts.nPass(geneExpr, deconMatrices, method = "DCQ")
```

Arguments

`geneExpr`	The gene expression matrix
`deconMatrices`	The results from spillToConvergence()
`method`	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)

Value

An estimate of cell counts

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

deconMatrices <- spillToConvergence(sigMatrix=smallLM22, geneExpr=fullLM22, nPasses=10)
cellCounts <- estCellCounts.nPass(geneExpr=fullLM22, deconMatrices=deconMatrices, method='DCQ')
```

`estCellPercent` *Wrapper for deconvolution methods*

Description

A wrapper function to call any of the estCellPercent functions

Usage

```
estCellPercent(refExpr, geneExpr, method = "DCQ", ...)
```

Arguments

refExpr	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
geneExpr	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)
...	Parameters for estCellPercent.X (e.g. number_of_repeats for .DCQ)

Value

A matrix with cell type estimates for each samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent(refExpr=smallLM22, geneExpr=fullLM22)
```

---

estCellPercent.DCQ *DCQ Deconvolution*

Description

Use DCQ to estimate the cell count percentage Requires installation of package 'ComICS' To Do: Also report the standard deviation as a confidence metric

Usage

```
estCellPercent.DCQ(
  refExpr,
  geneExpr,
  marker_set = NULL,
  number_of_repeats = 10,
```

```
  alpha = 0.05,
  lambda = 0.2
)
```

Arguments

refExpr	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
geneExpr	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
marker_set	data frames of one column, that includes a preselected list of genes that likely discriminate well between the immune-cell types given in the reference data. (DEFAULT: NULL, i.e. one for each gene in the refExpr)
number_of_repeats	using one repeat will generate only one output model. Using many repeats, DCQ calculates a collection of models, and outputs the average and standard deviation for each predicted relative cell quantity. (DEFAULT: 1)
alpha	The elasticnet mixing parameter, with 0 <= alpha <= 1. alpha=1 is the lasso penalty, and alpha=0 the ridge penalty. (DEFAULT: 0.05)
lambda	A minimum value for the elastic net lambda parameter (DEFAULT: 0.2)

Value

A matrix with cell type estimates for each samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.DCQ(refExpr=smallLM22, geneExpr=fullLM22)
```

`estCellPercent.DeconRNASeq` *DeconRNASeq deconvolution*

Description

Use DeconRNASeq to estimate the cell count percentage Performs with similar effectiveness as DCQ, but identifies different proportions of cell-types Requires installation of package 'DeconRNASeq': source("https://bioconductor.org/biocLite.R") biocLite("DeconRNASeq")

<joseph.szustakowski@novartis.com> TGJDS (2013). DeconRNASeq: Deconvolution of Heterogeneous Tissue Samples for mRNA-Seq data. R package version 1.18.0.

cellEst <- estCellPercent.DeconRNASeq(refExpr, geneExpr, marker_set=NULL)

Usage

```
estCellPercent.DeconRNASeq(refExpr, geneExpr, marker_set = NULL)
```

Arguments

`refExpr`	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
`geneExpr`	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
`marker_set`	data frames of one column, that includes a preselected list of genes that likely discriminate well between the immune-cell types given in the reference data. (DEFAULT: NULL, i.e. one for each gene in the refExpr)

Value

A matrix with cell type estimates for each samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.DeconRNASeq(refExpr=smallLM22, geneExpr=fullLM22)
```

`estCellPercent.nnls` *Non-negative least squares deconvolution*

Description

Use non-negative least squares regression to deconvolve a sample This is going to be to simple to be useful This might be more interesting if I used non-positive least squares to detect 'other'

Usage

```
estCellPercent.nnls(refExpr, geneExpr)
```

Arguments

`refExpr`	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
`geneExpr`	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.

Value

A matrix with cell type estimates for each samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.nnls(refExpr=smallLM22, geneExpr=fullLM22)
```

`estCellPercent.proportionsInAdmixture` *WGCNA::proportionsInAdmixture deconvolution*

Description

Use R function proportionsInAdmixture to estimate the cell count percentage Uses the 'WGCNA' package

cellEst <- estCellPercent.proportionsInAdmixture(refExpr)

Usage

```
estCellPercent.proportionsInAdmixture(refExpr, geneExpr, marker_set = NULL)
```

Arguments

`refExpr`	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
`geneExpr`	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
`marker_set`	data frames of one column, that includes a preselected list of genes that likely discriminate well between the immune-cell types given in the reference data. (DEFAULT: NULL, i.e. one for each gene in the refExpr)

Value

A matrix with cell type estimates for each samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.proportionsInAdmixture(refExpr=smallLM22, geneExpr=fullLM22)
```

estCellPercent.spillOver *Estimate cell percentage from spillover*

Description

Use a spillover matrix to deconvolve a samples

Usage

```
estCellPercent.spillOver(spillExpr, refExpr, geneExpr, method = "DCQ", ...)
```

Arguments

spillExpr	A spill over matrix, as calculated by buildSpilloverMat(). (e.g. LM22.spillover.csv.gz)
refExpr	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
geneExpr	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)
...	Parameters for estCellPercent.X (e.g. number_of_repeats for .DCQ)

Value

a matrix of estimate cell type percentages in samples

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

spillover <- buildSpilloverMat(refExpr=smallLM22, geneExpr=fullLM22)
cellEst <- estCellPercent.spillOver(spillExpr=spillover, refExpr=smallLM22, geneExpr=fullLM22)
```

`estCellPercent.svmdecon` *SVMDECON deconvolution*

Description

Use SVMDECON to estimate the cell count percentage Performs considerably worse in deconvolution than DCQ

cellEst <- estCellPercent.svmdecon(refExpr, geneExpr)

Usage

```
estCellPercent.svmdecon(
  refExpr,
  geneExpr,
  marker_set = NULL,
  useOldVersion = F,
  progressBar = T
)
```

Arguments

`refExpr`	a data frame representing immune cell expression profiles. Each row represents an expression of a gene, and each column represents a different immune cell type. colnames contains the name of each immune cell type and the rownames includes the genes' symbol. The names of each immune cell type and the symbol of each gene should be unique. Any gene with missing expression values must be excluded.
`geneExpr`	a data frame representing RNA-seq or microarray gene-expression profiles of a given complex tissue. Each row represents an expression of a gene, and each column represents a different experimental sample. colnames contain the name of each sample and rownames includes the genes' symbol. The name of each individual sample and the symbol of each gene should be unique. Any gene with missing expression values should be excluded.
`marker_set`	data frames of one column, that includes a preselected list of genes that likely discriminate well between the immune-cell types given in the reference data. (DEFAULT: NULL, i.e. one for each gene in the refExpr)
`useOldVersion`	Set the TRUE to 2^ the data (DEFAULT: FALSE)
`progressBar`	Set to TRUE to show a progress bar (DEFAULT: TRUE)

Value

A matrix with cell type estimates for each samples #This toy example library(ADAPTS) fullLM22 <- ADAPTS::LM22[1:30, 1:4] smallLM22 <- fullLM22[1:25,]

cellEst <- estCellPercent.svmdecon(refExpr=smallLM22, geneExpr=fullLM22)

getF1mcc *Get f1 / mcc*

Description

Get f1 / mcc and other accuracy measurements for binary predictions. Provide either an estimate and reference vector e.g. getF1mcc(estimate, reference) Or TPs, FPs, etc. e.g. getF1mcc(tps=3, fps=4, tns=7, fns=2)

Usage

```
getF1mcc(
  estimate = NULL,
  reference = NULL,
  tps = NULL,
  fps = NULL,
  tns = NULL,
  fns = NULL
)
```

Arguments

estimate	A binary vector of predictions
reference	a binary vector of actual values
tps	The number of TPs
fps	The number of FPs
tns	The number of TNs
fns	The number of FNs

Value

A vector with sensitivity, specificity, fpr, fdr, f1, agreement, p.value, mcc, and mcc.p

Examples

```
estimates <- sample(c(runif(8), 0 ,0))
reference <- sample(c(runif(7), 0 , 0, 0))
accuracyStats <- getF1mcc(estimate=estimates>0, reference=reference>0)
```

getLM22cells *LM22 look up table*

Description

Load a map of cell type names

Usage

```
getLM22cells()
```

Value

a map of cell types names

Examples

```
cellMap <- getLM22cells()
```

gListFromRF *Build a gList using random forest*

Description

Use ranger to select features and build a genesInSeed gene matrix

Usage

```
gListFromRF(trainSet, oneCore = FALSE)
```

Arguments

trainSet	Each row is a gene, and each column is an example of a particular cell type, e.g. ADAPTS::scSample(trainSet, groupSize=30)
oneCore	SEt to TRUE to disable multicore (DEFAULT: FALSE)

Value

A cell specific geneList for ADAPTS::AugmentSigMatrix()

Examples

```
library(ADAPTS)
ct1 <- runif(1000, 0, 100)
ct2 <- runif(1000, 0, 100)
dataMat <- cbind(ct1, ct1, ct1, ct1, ct1, ct1, ct2, ct2, ct2, ct2)
rownames(dataMat) <- make.names(rep('gene', nrow(dataMat)), unique=TRUE)
noise <- matrix(runif(nrow(dataMat)*ncol(dataMat), -2, 2), nrow = nrow(dataMat), byrow = TRUE)
dataMat <- dataMat + noise
gList <- gListFromRF(trainSet=dataMat, oneCore=TRUE)
```

---

hierarchicalClassify *Hierarchical Deconvolution*

Description

Deconvolve cell types based on clusters detected by an n-pass spillover matrix

Usage

```
hierarchicalClassify(
  sigMatrix,
  geneExpr,
  toPred,
  hierarchData = NULL,
  pdfDir = tempdir(),
  oneCore = FALSE,
  nPasses = 100,
  remZinf = TRUE,
  method = "DCQ",
  useRF = TRUE,
  incNonCluster = TRUE
)
```

Arguments

sigMatrix	The deconvolution matrix, e.g. LM22 or MGSM27
geneExpr	The source gene expression matrix used to calculate sigMatrix
toPred	The gene expression to ultimately deconvolve
hierarchData	The results of hierarchicalSplit OR hierarchicalSplit.sc (DEFAULT: NULL, ie hierarchicalSplit)
pdfDir	A fold to write the pdf file to (DEFAULT: tempdir())
oneCore	Set to TRUE to disable parallelization (DEFAULT: FALSE)
nPasses	The maximum number of iterations for spillToConvergence (DEFAULT: 100)
remZinf	Set to TRUE to remove any ratio with zero or infinity when generating gList (DEFAULT: FALSE)

method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)
useRF	Set to TRUE to use ranger random forests to build the seed matrix (DEFAULT: TRUE)
incNonCluster	Set to TRUE to include a 'nonCluster' in each of the sub matrices (DEFAULT: TRUE)

Value

a matrix of cell counts

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

cellCounts <- hierarchicalClassify(sigMatrix=smallLM22, geneExpr=fullLM22, toPred=fullLM22,
    oneCore=TRUE, nPasses=10, method='DCQ')
```

---

hierarchicalSplit *Build hierarchical cell clusters.*

Description

Attempt to deconvolve cell types by building a hierarchy of cell types using spillToConvergence to determine cell types that are not signficantly different. First deconvolve those clusters of cell types. Deconvolution matrices are then built to separate the cell types that formerly could not be separated.

Usage

```
hierarchicalSplit(
  sigMatrix,
  geneExpr,
  oneCore = FALSE,
  nPasses = 100,
  deconMatrices = NULL,
  remZinf = TRUE,
  method = "DCQ",
  useRF = TRUE,
  incNonCluster = TRUE
)
```

Arguments

sigMatrix	The deconvolution matrix, e.g. LM22 or MGSM27
geneExpr	The source gene expression matrix used to calculate sigMatrix
oneCore	Set to TRUE to disable parallelization (DEFAULT: FALSE)
nPasses	The maximum number of iterations for spillToConvergence (DEFAULT: 100)
deconMatrices	Optional pre-computed results from spillToConvergence (DEFAULT: NULL)
remZinf	Set to TRUE to remove any ratio with zero or infinity when generating gList (DEFAULT: FALSE)
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)
useRF	Set to TRUE to use ranger random forests to build the seed matrix (DEFAULT: TRUE)
incNonCluster	Set to TRUE to include a 'nonCluster' in each of the sub matrices (DEFAULT: TRUE)

Value

A list of clusters and a list of signature matrices for breaking those clusters

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

clusters <- hierarchicalSplit(sigMatrix=smallLM22, geneExpr=fullLM22, oneCore=TRUE, nPasses=10,
    deconMatrices=NULL, remZinf=TRUE, method='DCQ', useRF=TRUE, incNonCluster=TRUE)
```

Licenses *Licenses required by Celgene legal*

Description

This software is covered by the MIT license. Celgene legal thought it was wise to break the license up into the two license files included in this list.

Usage

```
data("Licenses")
```

Format

A data frame with 0 observations on the following 2 variables.

x a numeric vector

y a numeric vector

Source

https://www.r-project.org/Licenses/MIT

Examples

```
data(Licenses)
str(Licenses)
```

LM22 *Leukocyte 22 data matrix*

Description

Newman et al.'s 2015 22 leukocyte signature matrix.

Usage

```
data("LM22")
```

Format

A data frame with 547 observations on the following 22 variables.

`B.cells.naive` a numeric vector

`B.cells.memory` a numeric vector

`Plasma.cells` a numeric vector

`T.cells.CD8` a numeric vector

`T.cells.CD4.naive` a numeric vector

`T.cells.CD4.memory.resting` a numeric vector

`T.cells.CD4.memory.activated` a numeric vector

`T.cells.follicular.helper` a numeric vector

`T.cells.regulatory..Tregs.` a numeric vector

`T.cells.gamma.delta` a numeric vector

`NK.cells.resting` a numeric vector

`NK.cells.activated` a numeric vector

`Monocytes` a numeric vector

`Macrophages.M0` a numeric vector

`Macrophages.M1` a numeric vector

`Macrophages.M2` a numeric vector

`Dendritic.cells.resting` a numeric vector

`Dendritic.cells.activated` a numeric vector

`Mast.cells.resting` a numeric vector

`Mast.cells.activated` a numeric vector

`Eosinophils` a numeric vector

`Neutrophils` a numeric vector

Source

Newman, A. M. et al. Robust enumeration of cell subsets from tissue expression profiles. Nat. Methods 12, 453–457 (2015). https://media.nature.com/original/nature-assets/nmeth/journal/v12/n5/extref/nmeth.3337-S2.xls

Examples

```
data(LM22)
heatmap(as.matrix(LM22))
```

`loadMGSM27` *Load MGSM27*

Description

Load the MGSM27 signature matrix

Usage

```
loadMGSM27()
```

Value

The MGSM27 signature matrix from Identifying a High-risk Cellular Signature in the Multiple Myeloma Bone Marrow Microenvironment

Examples

```
MGSM27 <- loadMGSM27()
```

`loadModMap` *LM22 to xCell LUT*

Description

Load the LM22 xCell map

Usage

```
loadModMap()
```

Value

A map between xCell cell type names and LM22 cell type names

Examples

```
xcellMap <- loadModMap()
```

MGSM27 *Myeloma Genome Signature Matrix 27*

Description

Newman et al's 2015 plus 5 myeloma specific cell types. Osteoclasts, Adipocytes, Osteoblasts, Multiple Myeloma Plasma Cells, and Plasma Memory Cells

Usage

```
data("MGSM27")
```

Format

A data frame with 601 observations on the following 27 variables.

`B.cells.naive` a numeric vector

`B.cells.memory` a numeric vector

`Plasma.cells` a numeric vector

`T.cells.CD8` a numeric vector

`T.cells.CD4.naive` a numeric vector

`T.cells.CD4.memory.resting` a numeric vector

`T.cells.CD4.memory.activated` a numeric vector

`T.cells.follicular.helper` a numeric vector

`T.cells.regulatory..Tregs.` a numeric vector

`T.cells.gamma.delta` a numeric vector

`NK.cells.resting` a numeric vector

`NK.cells.activated` a numeric vector

`Monocytes` a numeric vector

`Macrophages.M0` a numeric vector

`Macrophages.M1` a numeric vector

`Macrophages.M2` a numeric vector

`Dendritic.cells.resting` a numeric vector

`Dendritic.cells.activated` a numeric vector

`Mast.cells.resting` a numeric vector

`Mast.cells.activated` a numeric vector

`Eosinophils` a numeric vector

`Neutrophils` a numeric vector

`MM.plasma.cell` a numeric vector

`osteoblast` a numeric vector

`osteoclast` a numeric vector

`PlasmaMemory` a numeric vector

`adipocyte` a numeric vector

Details

MGSM27 as constructed for Identifying a High-risk Cellular Signature in the Multiple Myeloma Bone Marrow Microenvironment.

Source

https://www.ebi.ac.uk/arrayexpress/experiments/E-MTAB-3732/ https://www.ebi.ac.uk/arrayexpress/experiments/E-MEXP-3711/ https://www.ebi.ac.uk/arrayexpress/experiments/E-MTAB-4152/

Examples

```
data(MGSM27)
heatmap(as.matrix(MGSM27))
```

---

missForest.par *Use parallel missForest to impute missing values.*

Description

This wrapper is helpful because missForest crashes if you have more cores than variables. This will default to no parellelization for Windows

newMatrix <- missForest.par(dataMat)

Usage

```
missForest.par(dataMat, parallelize = "variables")
```

Arguments

dataMat	Columns are features, Rows examples. The data with NA values. 'xmis' in missForest
parallelize	split on 'forests' or 'variables' (DEFAULT: 'variables')

Value

a matrix including imputed values

Examples

```
library(ADAPTS)
LM22 <- ADAPTS::LM22
LM22[2,3] <- as.numeric(NA) #Make some missing data to impute
LM22.imp <- missForest.par(LM22)
```

plotKappas *Plot condition numbers*

Description

Plot the condition numbers during the growing and shrinking of signature matrices.

bonusPoints <- data.frame(legText = c('Unagumented Signature Matrix', 'Minimum Smoothed Condition Number', 'Best Augmented Signature Matrix'), pchs = c('o', 'x', 'x'), cols = c('red', 'purple', 'blue'), kappa = c(10, 15, 20), nGene = c(5, 10, 15))

Usage

```
plotKappas(
  kappas,
  nGenes,
  smData = NULL,
  titleStr = "Shrink Signature Matrix",
  bonusPoints = NULL,
  maxCond = 100
)
```

Arguments

kappas	The condition numbers to plot
nGenes	The number of genes associated with each kapp
smData	Smoothed data to plot as a green line (DEFAULT: NULL)
titleStr	The title of the plot (DEFAULT: 'Shrink Signature Matrix')
bonusPoints	Set to plot additional points on the plot, see description (DEFAULT: NULL)
maxCond	Cap the condition number to maxCond (DEFAULT: 100)

Value

a matrix including imputed values

Examples

```
nGenes <- 1:300
kappas <- log(abs(nGenes-250))
kappas[is.infinite(kappas)] <- 0
kappas <- kappas+runif(300, 0, 1)
smData <- stats::smooth(kappas)
bonusPoints <- data.frame(legText = 'Minimum Smoothed ', pchs='x', cols='purple',
kappa=min(smData), nGenes=nGenes[which.min(smData)])
plotKappas(kappas=kappas, nGenes=nGenes, smData=smData, bonusPoints=bonusPoints, maxCond=100)
```

rankByT *Rank genes for each cell type*

Description

Use a t-test to rank to features for each cell type

gList <- rankByT(geneExpr, qCut=0.3)

Usage

```
rankByT(
  geneExpr,
  qCut = 0.3,
  oneCore = FALSE,
  secondPval = TRUE,
  remZinf = FALSE,
  reqRatGT1 = FALSE
)
```

Arguments

geneExpr	The gene expression data
qCut	(DEFAULT: 0.3)
oneCore	Set to TRUE to disable paralellization (DEFAULT: FALSE)
secondPval	Set to TRUE to use p-Values as a second sort criteria (DEFAULT: TRUE)
remZinf	Set to TRUE to remove any ratio with zero or infinity. Good for scRNAseq. (DEFAULT: FALSE)
reqRatGT1	Set to TRUE to remove any gene with a ratio with less than 1. Good for scRNAseq. (DEFAULT: FALSE)

Value

a list of cell types with data frames ranking genes

Examples

```
#This toy example treats the LM22 deconvolution matrix as if it were all of the data
#  For a real example, look at the vignette or comments in exprData, fullLM22, small LM22
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:200, 1:8]
#Make a fake signature matrix out of 100 genes and the first 8 cell types
smallLM22 <- fullLM22[1:100, 1:8]

#Make fake data representing two replicates of purified Mast.cells
exprData <- ADAPTS::LM22[1:200, c("Mast.cells.resting","Mast.cells.activated")]
colnames(exprData) <- c("Mast.cells", "Mast.cells")
```

```
#Fake source data with replicates for all purified cell types.
#  Note in this fake data set, many cell types have exactly one replicate
fakeAllData <- cbind(fullLM22, as.data.frame(exprData))
gList <- rankByT(geneExpr = fakeAllData, qCut=0.3, oneCore=TRUE, reqRatGT1=FALSE)
```

`remakeLM22p` *Make an Augmented Signature Matrix*

Description

With the ADAPTSdata packge, it will use the full LM22 data matrix and add a few additional genes to cover osteoblasts, osteoclasts, Plasma.memory, MM. In many ways this is just a convenient wrapper for AugmentSigMatrix that calculates and caches a gList.

Usage

```
remakeLM22p(
  exprData,
  fullLM22,
  smallLM22 = NULL,
  plotToPDF = TRUE,
  condTol = 1.01,
  postNorm = TRUE,
  autoDetectMin = FALSE,
  pdfDir = tempdir(),
  oneCore = FALSE
)
```

Arguments

`exprData`	The gene express data to use to augment LM22, e.g. ADAPTSdata::addMGSM27
`fullLM22`	LM22 data with all genes. Available in ADAPTSdata2::fullLM22
`smallLM22`	The small LM22 matrix, if it includes new cell types in exprData those will not be overwritten (DEFAULT: NULL, i.e. buildLM22plus(useLM22genes = TRUE)
`plotToPDF`	TRUE: pdf, FALSE: standard display (DEFAULT: TRUE)
`condTol`	The tolerance in the reconstruction algorithm. 1.0 = no tolerance, 1.05 = 5% tolerance (DEFAULT: 1.01)
`postNorm`	Set to TRUE to normalize new signatures to match old signatures. To Do: Redo Kappa curve? (DEFAULT: TRUE)
`autoDetectMin`	Set to true to automatically detect the first local minima. GOOD PRELIMINARY RESULTS (DEAFULT: FALSE)
`pdfDir`	A fold to write the pdf file to if plotToPDF=TRUE (DEFAULT: tempdir())
`oneCore`	Set to TRUE to disable parallelization (DEFAULT: FALSE)

Value

a cell type signature matrix

Examples

```
#This toy example treats the LM22 deconvolution matrix as if it were all of the data
#  For a real example, look at the vignette or comments in exprData, fullLM22, small LM22
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:200, 1:8]
#Make a fake signature matrix out of 100 genes and the first 8 cell types
smallLM22 <- fullLM22[1:100, 1:8]

#Make fake data representing two replicates of purified Mast.cells
exprData <- ADAPTS::LM22[1:200, c("Mast.cells.resting","Mast.cells.activated")]
colnames(exprData) <- c("Mast.cells", "Mast.cells")
newSig <- remakeLM22p(exprData=exprData, fullLM22=fullLM22, smallLM22=smallLM22,
    plotToPDF=FALSE, oneCore=TRUE)
```

---

scSample *Build groupSize pools according to cellIDs*

Description

This function is intended to collapse many single cells into 3 (groupsize) groups with the average count across all cells in each of the groups. These groups can then be used to perform a t-test (for example) between the 3 groups of CellX with 3 groups of CellY

Usage

```
scSample(
  RNAcounts,
  cellIDs = colnames(RNAcounts),
  groupSize = 3,
  randomize = TRUE
)
```

Arguments

RNAcounts	The single cell matrix
cellIDs	A vector will cell types for each column in scCountMatrix (DEFAULT: colnames(RNAcounts))
groupSize	The number of sets to break it up into (DEFAULT: 3)
randomize	Set to TRUE to randomize the sets (DEFAULT: TRUE)

Value

a list with a multiple sets

Examples

```
RNAcounts <- matrix(0, nrow=10, ncol=100)
rownames(RNAcounts) <- make.names(rep('Gene', nrow(RNAcounts)), unique=TRUE)
colnames(RNAcounts) <- make.names(c('CellX', rep('CellY', 39),
rep('CellZ', 30), rep('CellB', 30)), unique=TRUE)
RNAcounts[, grepl('CellY', colnames(RNAcounts))] <- 1
RNAcounts[, grepl('CellZ', colnames(RNAcounts))] <- 2
RNAcounts[, grepl('CellB', colnames(RNAcounts))] <- 3
scSample(RNAcounts, groupSize=3)
```

---

shrinkByKappa *Calculate conditions numbers for signature subsets*

Description

Remove genes by chunks by picking those the most improve the condition number. Will set any infinite condition numbers to max(kappas[!is.infinite(kappas)])+1 Return the condition numbers with their gene lists

Usage

```
shrinkByKappa(
  sigMatrix,
  numChunks = NULL,
  verbose = TRUE,
  plotIt = TRUE,
  singleCore = FALSE,
  fastStop = TRUE
)
```

Arguments

sigMatrix	The original signature matrix
numChunks	The number of groups of genes to remove (DEFAULT: NULL)
verbose	Print out the current chunk as is it's being calculated (DEFAULT: NULL)
plotIt	The title of the plot (DEFAULT: TRUE)
singleCore	Set to FALSE to use multiple cores to calculate condition numbers (DEFAULT: FALSE)
fastStop	Halt early when the condition number changes by less than 1 for 3 iterations (DEFAULT: FALSE)

Value

A list with condition numbers and gene lists

Examples

```
library(ADAPTS)
LM22 <- ADAPTS::LM22
sigGenesList <- shrinkByKappa(sigMatrix=LM22[1:100,1:5], numChunks=4,
verbose=FALSE, plotIt=FALSE, singleCore=TRUE, fastStop=TRUE)
```

---

shrinkSigMatrix *Shrink a signature matrix*

Description

Use shrinkByKappa and automatic minima detection to reduce a signature matrix. Select the new signature matrix with the minima and the maximum number of genes. There is an inherent difficult in that the condition number will tend to have a second peak at a relatively small number of genes, and then crash so that smallest condition number has more or less one gene.

By default, the algorithm will tend to pick the detected minima with the largest nubmer of genes. aggressiveMin=TRUE will try to find the minimum number of genes that has more genes than the maxima at the smallest number of genes

Usage

```
shrinkSigMatrix(
  sigMatrix,
  numChunks = 100,
  verbose = FALSE,
  plotIt = FALSE,
  aggressiveMin = TRUE,
  sigGenesList = NULL,
  singleCore = FALSE,
  fastStop = TRUE
)
```

Arguments

sigMatrix	The original signature matrix
numChunks	The number of groups of genes to remove. NULL is all genes (DEFAULT: 100)
verbose	Print out the current chunk as is it's being calculated (DEFAULT: NULL)
plotIt	Set to TRUE to plot (DEFAULT: FALSE)
aggressiveMin	Set to TRUE to aggresively seek the smallest number of genes (DEFAULT: TRUE)
sigGenesList	Set to use precomputed results from shrinkByKappa (DEFAULT: NULL)
singleCore	Set to FALSE to use multiple cores to calculate condition numbers (DEFAULT: FALSE)
fastStop	Halt early when the condition number changes by less than 1 for 3 iterations (DEFAULT: TRUE)

Value

A list with condition numbers and gene lists

Examples

```
library(ADAPTS)
LM22 <- ADAPTS::LM22
newSigMat <- shrinkSigMatrix(sigMatrix=LM22[1:100,1:5], numChunks=4, verbose=FALSE,
plotIt=FALSE, aggressiveMin=TRUE, sigGenesList=NULL, singleCore=TRUE, fastStop=FALSE)
```

---

spillToConvergence *Spillover to convergence*

Description

Build an n-pass spillover matrix, continuing until the results converge into clusters of cell types

deconMatrices <- spillToConvergence(sigMatrix, geneExpr, 100, FALSE, TRUE)

Usage

```
spillToConvergence(
  sigMatrix,
  geneExpr,
  nPasses = 100,
  plotIt = FALSE,
  imputNAs = FALSE,
  method = "DCQ"
)
```

Arguments

sigMatrix	The deconvolution matrix, e.g. LM22 or MGSM27
geneExpr	The source gene expression matrix used to calculate sigMatrix
nPasses	The maximum number of iterations (DEFAULT: 100)
plotIt	Set to TRUE to plot it (DEFAULT: FALSE)
imputNAs	Set to TRUE to imput genes with missing values & cache the imputed. FALSE will just remove them (DEFAULT: FALSE)
method	One of 'DCQ', 'SVMDECON', 'DeconRNASeq', 'proportionsInAdmixture', 'nnls' (DEFAULT: DCQ)

Value

A list of signature matrices

Examples

```
#This toy example
library(ADAPTS)
fullLM22 <- ADAPTS::LM22[1:30, 1:4]
smallLM22 <- fullLM22[1:25,]

deconMatrices <- spillToConvergence(sigMatrix=smallLM22, geneExpr=fullLM22, nPasses=10, plotIt=TRUE)
```

`splitSCdata` *Split a single cell dataset into multiple sets*

Description

Take a matrix of single cell data with genes as rows and each column corresponding to a single cells. Break it up into rougly equal subsets, taking care to make sure that each cell type is represented in each set if possible

Usage

```
splitSCdata(
  RNAcounts,
  cellIDs = colnames(RNAcounts),
  numSets = 3,
  verbose = TRUE,
  randomize = TRUE
)
```

Arguments

`RNAcounts`	The single cell matrix
`cellIDs`	A vector will cell types for each column in scCountMatrix (DEFAULT: colnames(RNAcounts))
`numSets`	The number of sets to break it up into (DEFAULT: 3)
`verbose`	Set to TRUE to print cell counts as it goes (DEFAULT: TRUE)
`randomize`	Set to TRUE to randomize the sets (DEFAULT: TRUE)

Value

a list with a multiple sets

Examples

```
RNAcounts <- matrix(0, nrow=10, ncol=30)
rownames(RNAcounts) <- make.names(rep('Gene', nrow(RNAcounts)), unique=TRUE)
colnames(RNAcounts) <- make.names(c('CellX', rep('CellY', 9),
rep('CellZ', 10), rep('CellB', 10)), unique=TRUE)
RNAcounts[, grepl('CellY', colnames(RNAcounts))] <- 1
RNAcounts[, grepl('CellZ', colnames(RNAcounts))] <- 2
RNAcounts[, grepl('CellB', colnames(RNAcounts))] <- 3
splitSCdata(RNAcounts, numSets=3)
```

SVMDECON *Support vector machine deconvolution*

Description

Use SVMDECONV to estimate the cell count percentage David L Gibbs, dgibbs@systemsbiology.org June 9, 2017

v-SVR is applied with a linear kernel to solve for f, and the best result from three values of v = 0.25, 0.5, 0.75 is saved, where 'best' is defined as the lowest root mean squared error between m and the deconvolution result, f x B.

Our current implementation executes v-SVR using the 'svm' function in the R package, 'e1071'.

w2 <- SVMDECON(m, B)

Usage

```
SVMDECON(m, B)
```

Arguments

m	a matrix represenging the mixture (genes X 1 sample)
B	a matrix representing the references (genes X cells), m should be subset to match B

Value

A matrix with cell type estimates for each samples

`weightNorm` *SVMDECONV helper function*

Description

Use weightNorm to normalize the SVM weights. Used for SVMDECONV

w1 <- weightNorm(w)

Usage

```
weightNorm(w)
```

Arguments

`w`	The weight vector from fitting an SVM, something like something like t(fit1$coefs) %*% fit1$SV, where fit comes from <- svm(m~B, nu=0.25, kernel="linear"))

Value

a weight vector

Index

∗ **datasets**
Licenses, 21
LM22, 22
MGSM27, 24

AugmentSigMatrix, 3

buildSeed, 4
buildSpilloverMat, 6

calcAcc, 6
clustWspillOver, 7
collapseCellTypes, 8

estCellCounts.nPass, 9
estCellPercent, 9
estCellPercent.DCQ, 10
estCellPercent.DeconRNASeq, 12
estCellPercent.nnls, 13
estCellPercent.proportionsInAdmixture, 14
estCellPercent.spillOver, 15
estCellPercent.svmdecon, 16

getF1mcc, 17
getLM22cells, 18
gListFromRF, 18

hierarchicalClassify, 19
hierarchicalSplit, 20

Licenses, 21
LM22, 22
loadMGSM27, 23
loadModMap, 23

MGSM27, 24
missForest.par, 25

plotKappas, 26

rankByT, 27
remakeLM22p, 28

scSample, 29
shrinkByKappa, 30
shrinkSigMatrix, 31
spillToConvergence, 32
splitSCdata, 33
SVMDECON, 34

weightNorm, 35